

# Twisting singular solutions of Bethe's equations

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## Abstract

The Bethe equations for the periodic XXX and XXZ spin chains admit singular solutions, for which the corresponding eigenvalues and eigenvectors are ill-defined. We use a twist regularization to derive conditions for such singular solutions to be physical, in which case they correspond to genuine eigenvalues and eigenvectors of the Hamiltonian.

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# 1 Introduction

The periodic spin-1/2 isotropic Heisenberg (XXX) quantum spin chain, whose Hamiltonian is given by<sup>1</sup>

$$H = \frac{1}{4} \sum_{n=1}^N (\vec{\sigma}_n \cdot \vec{\sigma}_{n+1} - 1), \quad \vec{\sigma}_{N+1} \equiv \vec{\sigma}_1, \quad (1)$$

is well known to be solvable by Bethe ansatz: both the eigenvectors and the eigenvalues of the Hamiltonian can be expressed in terms of solutions of the Bethe equations [1, 2]

$$\left( \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}} \right)^N = \prod_{\substack{k \neq j \\ k=1}}^M \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}, \quad j = 1, \dots, M, \quad M = 0, 1, \dots, \frac{N}{2}. \quad (2)$$

Indeed, the eigenvectors are given in terms of the ‘‘Bethe roots’’  $\{\lambda_j\}$  by the Bethe vector

$$\prod_{j=1}^M B(\lambda_j) |0\rangle, \quad (3)$$

where  $B(\lambda)$  is a certain creation operator<sup>2</sup> and  $|0\rangle$  is the state with all  $N$  spins up; and the corresponding eigenvalues are given by

$$E = -\frac{1}{2} \sum_{j=1}^M \frac{1}{\lambda_j^2 + \frac{1}{4}}. \quad (4)$$

It is also well known that the Bethe equations admit so-called singular (or exceptional) solutions, for which the corresponding eigenvectors and eigenvalues are ill-defined. (See e.g.

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<sup>1</sup>We denote by  $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$  the standard Pauli spin matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

which act on a two-dimensional complex vector space  $V = \mathbb{C}^2$ . Moreover,  $\sigma_n^i$  denotes an operator on the  $N$ -fold tensor product space  $V^{\otimes N}$ , which acts as  $\sigma^i$  on the  $n^{\text{th}}$  copy of  $V$ , and as the identity operator otherwise

$$\sigma_n^i = \mathbb{I} \otimes \dots \otimes \mathbb{I} \otimes \overset{n}{\downarrow} \sigma^i \otimes \mathbb{I} \dots \otimes \mathbb{I},$$

where here  $\mathbb{I}$  denotes the  $2 \times 2$  identity matrix.

<sup>2</sup>We remind the reader that the monodromy matrix is given by [2]

$$T_a(\lambda) = L_{Na}(\lambda) \cdots L_{1a}(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix},$$

where the Lax operator is  $L_{na}(\lambda) = (\lambda - \frac{i}{2})\mathbb{I}_{na} + i\mathcal{P}_{na}$ , and  $\mathcal{P}$  is the permutation matrix on  $V \otimes V$ . The operator  $B(\lambda)$  serves as a creation operator for constructing the eigenstates of  $H$ , and has the property  $[B(\lambda), B(\lambda')] = 0$ . The transfer matrix  $t(\lambda) = \text{tr}_a T_a(\lambda) = A(\lambda) + D(\lambda)$  satisfies  $[t(\lambda), t(\lambda')] = 0$ , and therefore is the generator of commuting quantities  $H_n = \frac{i}{2} \frac{d^n}{d\lambda^n} \log t(\lambda)|_{\lambda=\frac{i}{2}}$ , with  $H = H_1 - \frac{N}{2}$ .

[3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14].) The simplest example occurs for  $M = 2$  and any  $N \geq 4$ , namely  $(\lambda_1, \lambda_2) = (i/2, -i/2)$ . To see that this is an exact solution, it is convenient to rewrite the Bethe equations (2) in polynomial form (see e.g. (10) below). The corresponding energy (4) is evidently ill-defined, and the corresponding eigenvector (3) can be shown to be null.

A general singular solution of the Bethe equations has the form

$$\left\{ \frac{i}{2}, -\frac{i}{2}, \lambda_3, \dots, \lambda_M \right\}, \quad (5)$$

where  $\lambda_3, \dots, \lambda_M$  are distinct and not equal to  $\pm i/2$ . A solution that does not contain  $\pm i/2$  is called regular. Note that the order of the Bethe roots does not matter, since the Bethe equations (2) as well as the eigenvectors (3) and eigenvalues (4) are invariant under any permutation of  $\{\lambda_1, \dots, \lambda_M\}$ .

It is important to recognize that there are two main types of singular solutions: **physical** singular solutions (which correspond to genuine eigenvalues and eigenvectors of the Hamiltonian), and **unphysical** singular solutions (which do not correspond to eigenvalues and eigenvectors of the Hamiltonian). The simplest example of the former is  $\pm i/2$  for  $N$  even, while the simplest example of the latter is  $\pm i/2$  for  $N$  odd.

We have argued in [14] that a general singular solution (5) is physical if  $\lambda_3, \dots, \lambda_M$  satisfy the following additional condition

$$\left[ -\prod_{j=3}^M \left( \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}} \right) \right]^N = 1. \quad (6)$$

For the case  $M = 2$ , this condition reduces to the requirement (already noted above) that  $N$  should be even.

This condition was used in [15] to explicitly demonstrate the completeness of the solutions of Bethe's equations up to  $N = 14$ . That is, the number of regular solutions plus the number of physical singular solutions (i.e., those singular solutions that satisfy (6)) exactly coincides with the number needed to account for all  $2^N$  eigenstates of the model. For further discussions of the completeness problem, see for example [1, 2, 10, 16, 17, 18, 19, 20, 21, 22, 23, 24].

For the integrable spin- $s$  XXX chain, a generalization of (6) was derived and used to investigate completeness in [25]. For related recent developments, see [26, 27, 28].

The derivation of the constraint (6) in [14] (and similarly of its spin- $s$  generalization in [25]) relies on regularizing the singular solution (5) by replacing the first two roots by

$$\lambda_1 = \frac{i}{2} + \epsilon + c\epsilon^N, \quad \lambda_2 = -\frac{i}{2} + \epsilon, \quad (7)$$

where  $\epsilon$  is a small parameter, and  $c$  is a constant that is still to be determined. This way of regularizing a singular solution was considered previously in [3, 8, 9, 10]. Requiring that the corresponding Bethe vector (constructed as in (3), except with a different normalization of the creation operators, namely  $B(\lambda) \mapsto (\lambda + \frac{i}{2})^{-N} B(\lambda)$ , which diverges at  $\lambda = -\frac{i}{2}$ ) be

an eigenvector of the transfer matrix in the limit  $\epsilon \rightarrow 0$  gives rise to two equations for the constant  $c$ , whose consistency implies (6).

The regularization scheme (7) may be rightly criticized as being somewhat unphysical and ad-hoc. Moreover, one can worry that a different choice of regularization could lead to a result different from (6). The primary motivation for the present work was to see whether this constraint could be derived using a different, and more physical, regularization.

An alternative regularization is to introduce a small diagonal twist angle  $\beta$  in the boundary conditions (see e.g. [4])

$$\begin{aligned}\sigma_{N+1}^x &= \cos \beta \sigma_1^x - \sin \beta \sigma_1^y, \\ \sigma_{N+1}^y &= \sin \beta \sigma_1^x + \cos \beta \sigma_1^y, \\ \sigma_{N+1}^z &= \sigma_1^z.\end{aligned}\tag{8}$$

This boundary condition evidently breaks the  $SU(2)$  symmetry down to  $U(1)$ , and reduces to periodic boundary conditions when  $\beta = 0$ .

This way of regularizing a singular solution was considered previously in [6, 11, 12, 13]. Moreover, such twists have been widely used in related contexts (see e.g. [12, 18, 19, 20, 29, 30, 31] and references therein). Like (7), the twist regularization (8) involves introducing an additional parameter; however, the latter regularization is arguably more physical, since its parameter has a physical meaning.

We show here that the constraint (6) can indeed be derived (in fact, more easily) using the twist (8) as a regulator. The argument easily generalizes to the case of arbitrary spin  $s$ , and also to the XXZ case.

## 2 XXX

For the spin-1/2 XXX spin chain with twisted boundary conditions (8), the Bethe equations are given by

$$\left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}\right)^N = e^{-i\beta} \prod_{\substack{k \neq j \\ k=1}}^M \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}, \quad j = 1, \dots, M, \tag{9}$$

which can be rewritten in polynomial form as

$$\left(\lambda_j + \frac{i}{2}\right)^N \prod_{\substack{k \neq j \\ k=1}}^M (\lambda_j - \lambda_k - i) = e^{-i\beta} \left(\lambda_j - \frac{i}{2}\right)^N \prod_{\substack{k \neq j \\ k=1}}^M (\lambda_j - \lambda_k + i), \quad j = 1, \dots, M. \tag{10}$$

We assume that, for small  $\beta$ , the roots  $\pm i/2$  of a physical singular solution (5) acquire

corrections of order  $\beta$ ,<sup>3</sup>

$$\begin{aligned}\lambda_1 &= \frac{i}{2} + c_1\beta + O(\beta^2), \\ \lambda_2 &= -\frac{i}{2} + c_2\beta + O(\beta^2),\end{aligned}\tag{11}$$

where  $c_1$  and  $c_2$  are some constants (independent of  $\beta$ ). The Bethe equations (10) for  $\lambda_1$  and  $\lambda_2$  are

$$\begin{aligned}\left(\lambda_1 + \frac{i}{2}\right)^N (\lambda_1 - \lambda_2 - i) \prod_{k=3}^M (\lambda_1 - \lambda_k - i) &= e^{-i\beta} \left(\lambda_1 - \frac{i}{2}\right)^N (\lambda_1 - \lambda_2 + i) \prod_{k=3}^M (\lambda_1 - \lambda_k + i), \\ \left(\lambda_2 + \frac{i}{2}\right)^N (\lambda_2 - \lambda_1 - i) \prod_{k=3}^M (\lambda_2 - \lambda_k - i) &= e^{-i\beta} \left(\lambda_2 - \frac{i}{2}\right)^N (\lambda_2 - \lambda_1 + i) \prod_{k=3}^M (\lambda_2 - \lambda_k + i).\end{aligned}$$

Substituting (11), one can see that these equations are satisfied to first order in  $\beta$  provided that

$$c_1 = c_2.\tag{12}$$

Forming the product of all  $M$  Bethe equations (9), we obtain

$$\left(\frac{\lambda_1 + \frac{i}{2}}{\lambda_1 - \frac{i}{2}} \frac{\lambda_2 + \frac{i}{2}}{\lambda_2 - \frac{i}{2}} \prod_{j=3}^M \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}\right)^N = e^{-iM\beta}.\tag{13}$$

Substituting (11) and (12) into (13) and taking the limit  $\beta \rightarrow 0$ , we arrive at the constraint (6)

$$\left[-\prod_{j=3}^M \left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}\right)\right]^N = 1.\tag{14}$$

This concludes our argument for the spin-1/2 XXX case. Of course,  $\{\lambda_3, \dots, \lambda_M\}$  must also obey

$$\left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}\right)^{N-1} \left(\frac{\lambda_j - \frac{3i}{2}}{\lambda_j + \frac{3i}{2}}\right) = \prod_{\substack{k \neq j \\ k=3}}^M \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}, \quad j = 3, \dots, M,\tag{15}$$

which follow from the Bethe equations (9) with  $j = 3, \dots, M$  after substituting (11) and taking  $\beta \rightarrow 0$ .

The constraint (14) can also be derived in a similar way using the original regularization (7) simply by substituting into (13) (with  $\beta = 0$ ) and taking the limit  $\epsilon \rightarrow 0$ . This argument (which was overlooked in [14]) evidently does not require the  $\epsilon\epsilon^N$  term in (7). However, this  $\epsilon\epsilon^N$  term is needed to construct the correct eigenvector.

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<sup>3</sup>The twisted equations (10) evidently still admit solutions with  $\pm i/2$  (i.e., without any  $\beta$ -dependent corrections). However, such singular solutions are unphysical.

In order to construct the eigenvector corresponding to a physical singular solution using the twist regularization, we expect (based on [14]) that it is necessary to determine the corrections of the singular solution up to order  $\beta^N$ , to renormalize the Bethe vector (3) by the factor  $1/\beta^N$ , and then take the limit  $\beta \rightarrow 0$ . The required corrections of the singular solution can be obtained (for given explicit values  $\{\lambda_j^{(0)}\}$  of  $\{\lambda_3, \dots, \lambda_M\}$  that satisfy (14) and (15)) by assuming that all the Bethe roots can be expanded in powers of  $\beta$ ,

$$\lambda_j = \lambda_j^{(0)} + \sum_{l=1}^N c_j^{(l)} \beta^l + O(\beta^{N+1}), \quad j = 1, \dots, M, \quad (16)$$

and solving the Bethe equations (10), (13) for the coefficients  $c_j^{(l)}$ . For example, for the simplest case  $(N, M) = (4, 2)$ , we find in this way

$$\begin{aligned} \lambda_1 &= \frac{i}{2} + \frac{\beta}{4} - \frac{\beta^3}{96} + \frac{i\beta^4}{256} + O(\beta^5), \\ \lambda_2 &= -\frac{i}{2} + \frac{\beta}{4} - \frac{\beta^3}{96} - \frac{i\beta^4}{256} + O(\beta^5). \end{aligned} \quad (17)$$

Moreover, we have verified by explicit computation that the vector

$$\lim_{\beta \rightarrow 0} \frac{1}{\beta^4} B(\lambda_1) B(\lambda_2) |0\rangle \quad (18)$$

is indeed proportional to the correct eigenvector  $[3, 5] \sum_{k=1}^4 (-1)^k S_k^- S_{k+1}^- |0\rangle$ .

## 2.1 Spin $s$

Similar arguments can be applied to the integrable spin- $s$  XXX chain with twisted boundary conditions, for arbitrary spin  $s = \frac{1}{2}, 1, \frac{3}{2}, \dots$ . The Bethe equations are given by

$$\left( \frac{\lambda_j + is}{\lambda_j - is} \right)^N = e^{-i\beta} \prod_{\substack{k \neq j \\ k=1}}^M \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}, \quad j = 1, \dots, M, \quad (19)$$

When  $\beta = 0$ , these equations have singular solutions of the form [25]

$$\{is, i(s-1), \dots, -i(s-1), -is, \lambda_{2s+2}, \dots, \lambda_M\}, \quad (20)$$

where all the roots are assumed to be distinct. That is, a singular solution contains an exact string of length  $2s+1$  centered at the origin.

We assume that, for small  $\beta$ , the roots  $\{is, i(s-1), \dots, -i(s-1), -is\}$  of a physical singular solution acquire corrections of order  $\beta$ ,

$$\lambda_k = i(s+1-k) + c_k \beta + O(\beta^2), \quad k = 1, 2, \dots, 2s+1, \quad (21)$$

where  $\{c_k\}$  are some constants. Substituting (21) into the first  $2s+1$  Bethe equations (i.e., Eq. (19) for  $j = 1, \dots, 2s+1$ ), we see that these equations are satisfied to first order in  $\beta$  provided that all the  $c_k$ 's are equal,

$$c_1 = c_2 = \dots = c_{2s+1}. \quad (22)$$

The product of all  $M$  Bethe equations (19) gives

$$\left( \frac{\lambda_1 + is}{\lambda_1 - is} \frac{\lambda_2 + is}{\lambda_2 - is} \cdots \frac{\lambda_{2s+1} + is}{\lambda_{2s+1} - is} \prod_{j=2s+2}^M \frac{\lambda_j + is}{\lambda_j - is} \right)^N = e^{-iM\beta}. \quad (23)$$

Substituting (21) and (22) into (23) and taking the limit  $\beta \rightarrow 0$ , we obtain the constraint

$$\left[ (-1)^{2s} \prod_{j=2s+2}^M \left( \frac{\lambda_j + is}{\lambda_j - is} \right) \right]^N = 1. \quad (24)$$

This necessary condition for the singular solution (20) to be physical, which is evidently a generalization of the  $s = 1/2$  result (14), was first obtained in [25] using instead a generalization of the regularization (7). Of course,  $\{\lambda_{2s+2}, \dots, \lambda_M\}$  must also obey

$$\left( \frac{\lambda_j + is}{\lambda_j - is} \right)^{N-1} \left( \frac{\lambda_j - i(s+1)}{\lambda_j + i(s+1)} \right) = \prod_{\substack{k \neq j \\ k=2s+2}}^M \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}, \quad j = 2s+2, \dots, M, \quad (25)$$

which follow from the Bethe equations (19) with  $j = 3, \dots, M$  after substituting (21) and taking  $\beta \rightarrow 0$ .

### 3 XXZ

For the spin-1/2 XXZ spin chain with twisted boundary conditions, the Bethe equations are given by

$$\left( \frac{\sinh(\lambda_j + \frac{\eta}{2})}{\sinh(\lambda_j - \frac{\eta}{2})} \right)^N = e^{-i\beta} \prod_{\substack{k \neq j \\ k=1}}^M \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)}, \quad j = 1, \dots, M, \quad (26)$$

where  $\eta$  is the anisotropy parameter, which we assume has a generic value (i.e.,  $q = e^\eta$  is not a root of unity). When  $\beta = 0$ , these equations have singular solutions of the form

$$\left\{ \frac{\eta}{2}, -\frac{\eta}{2}, \lambda_3, \dots, \lambda_M \right\}. \quad (27)$$

Repeating the same steps of our argument for the isotropic case, we conclude that a physical singular solution must satisfy the constraint

$$\left[ - \prod_{j=3}^M \frac{\sinh(\lambda_j + \frac{\eta}{2})}{\sinh(\lambda_j - \frac{\eta}{2})} \right]^N = 1, \quad (28)$$

as well as

$$\left( \frac{\sinh(\lambda_j + \frac{\eta}{2})}{\sinh(\lambda_j - \frac{\eta}{2})} \right)^{N-1} \frac{\sinh(\lambda_j - \frac{3\eta}{2})}{\sinh(\lambda_j + \frac{3\eta}{2})} = \prod_{\substack{k \neq j \\ k=3}}^M \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)}, \quad j = 3, \dots, M. \quad (29)$$

Similarly, for the spin- $s$  XXZ spin chain with twisted boundary conditions, the Bethe equations are given by

$$\left(\frac{\sinh(\lambda_j + s\eta)}{\sinh(\lambda_j - s\eta)}\right)^N = e^{-i\beta} \prod_{\substack{k \neq j \\ k=1}}^M \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)}, \quad j = 1, \dots, M. \quad (30)$$

When  $\beta = 0$ , these equations have singular solutions of the form

$$\{s\eta, (s-1)\eta, \dots, -(s-1)\eta, -s\eta, \lambda_{2s+2}, \dots, \lambda_M\}, \quad (31)$$

where again all the roots are assumed to be distinct. A physical singular solution of this form must satisfy the constraint

$$\left[(-1)^{2s} \prod_{j=2s+2}^M \frac{\sinh(\lambda_j + s\eta)}{\sinh(\lambda_j - s\eta)}\right]^N = 1, \quad (32)$$

as well as

$$\left(\frac{\sinh(\lambda_j + s\eta)}{\sinh(\lambda_j - s\eta)}\right)^{N-1} \frac{\sinh(\lambda_j - (s+1)\eta)}{\sinh(\lambda_j + (s+1)\eta)} = \prod_{\substack{k \neq j \\ k=2s+2}}^M \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)}, \quad j = 2s+2, \dots, M. \quad (33)$$

The constraint (28) and its generalization (32), which heretofore had not been written down, can also be straightforwardly derived using the alternative regularization (7) following [14] and [25].

## 4 Conclusion

We have argued that a twist regularization can be used to derive the constraints (14), (24), (28), (32) for singular solutions of the periodic XXX and XXZ spin chains to be physical. The fact that these constraints can be derived using two different regularizations suggests that they are independent of the choice of regularization. Indeed, the fact that these constraints appear already at first order in the regulator (instead of order  $N$ , as suggested by the original derivations [14, 25]) implies that they are robust.

Although the arguments presented here demonstrate only that these conditions are necessary, the arguments in [14] and [25] imply that these conditions are also sufficient for singular solutions to be physical. This conclusion is also supported by numerical evidence [15, 25]. The latter references also show that most of the solutions of the Bethe equations are unphysical singular solutions; hence, it is all the more important to have simple criteria for picking out from among the many singular solutions the few that are physical.

As noted in [3, 25], the Bethe equations for chains with  $s > 1/2$  can also have singular solutions with repeated roots that are physical. We expect that the twist regularization considered here can also be used to derive conditions for such “strange” singular solutions to be physical.



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